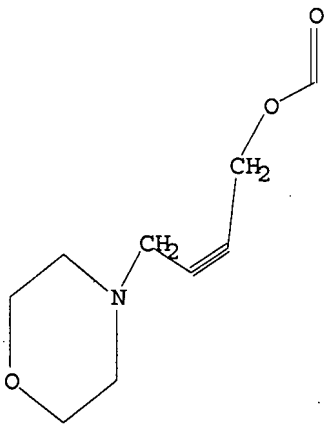
5-7 7-8 8-9 9-10 10-11 11-12 12-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 12-13
exact bonds :
5-7 7-8 8-9 9-10 10-11
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:32:18 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 34 TO ITERATE

100.0% PROCESSED 34 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 331 TO 1029
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 13:32:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 612 TO ITERATE

100.0% PROCESSED 612 ITERATIONS 64 ANSWERS
SEARCH TIME: 00.00.01

L3 64 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.10	172.31

FILE 'CAPLUS' ENTERED AT 13:32:28 ON 29 OCT 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 29 Oct 2007 VOL 147 ISS 19
FILE LAST UPDATED: 28 Oct 2007 (20071028/ED)

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=> s l3
L4 38 L3

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own work

L4 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1103763 CAPLUS
DOCUMENT NUMBER: 143:387062
TITLE: Preparation of water soluble 4-amino-2-butynyl esters having anticancer activity
INVENTOR(S): Salama, Zoser B.
PATENT ASSIGNEE(S): Germany
SOURCE: PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005095369	A1	20051013	WO 2004-EP2090	20040302
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1732909	A1	20061220	EP 2004-716240	20040302
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				

PRIORITY APPLN. INFO.: WO 2004-EP2090 W 20040302

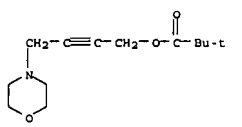
OTHER SOURCE(S): CASREACT 143:387062; MARPAT 143:387062

AB The present invention relates to water soluble 4-amino-2-butynyl or 4-(N-substituted amino)-2-butynyl esters (R1R2NCH2C.tplbond.CCH2O2R (I); variables defined below; e.g. 4-(morpholino)-2-butynyl acetate) and methods for production of said esters and the use of the esters for treatment of cancer. 4-Morpholino-2-butynyl acetate and 4-morpholino-2-butynyl pivalate show the highest antitumor activity amongst 8 examples of I and low toxicity to fibroblasts. For I: R is H, a straight-chained or branched, (un)saturated aliphatic radical with 1-20 C-atoms ((un)substituted ≥1 times by C1-C6-alkyl, C1-C6-alkoxy, halogen, epoxy, amino, mercapto, a Ph ring ((un)substituted ≥1 times by C1-C6-alkyl, C1-C6-alkoxy, hydroxy, epoxy, amino, mercapto or halogen)), a cycloalkyl group with 4 to 7 atoms ((un)substituted ≥1 times by C1-C6-alkyl, C1-C6-alkoxy, hydroxy, epoxy, amino, mercapto or halogen); R1 and R2 are joined to form a heterocyclic ring with 3 to 6 C-atoms, (un)substituted ≥1 times by C1-C6-alkyl, C1-C6-alkoxy, hydroxy, halogen, epoxy, amino, mercapto, whereby at least one C-atom can be replaced by O, S or N, or R1 and R2 = H, straight-chained or branched, (un)saturated aliphatic radical with 1-20 C-atoms, (un)substituted ≥1 times by C1-C6-alkyl, C1-C6-alkoxy, hydroxy, halogen, epoxy, amino, mercapto. Methods of prepn. are claimed and .apprx.10 example prepns. are included. For example, 4-(morpholino)-2-butynyl acetate was prepd. in 2 steps starting from propargyl alc. and acetic acid to give propargyl acetate, which underwent a Mannich condensation with paraformaldehyde and morpholine in the presence of CuCl.

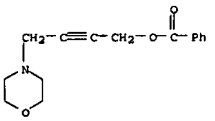
IT 35956-47-9P, 4-Morpholino-2-butynyl acetate 35956-48-0P, 4-(Morpholino)-2-butynyl pivalate 54757-85-6P, 4-(Morpholino)-2-butynyl benzoate 106087-86-9P, 4-(Morpholino)-2-butynyl propionate 866549-52-2P, 4-(Morpholino)-2-butynyl formate 866549-56-6P, 4-(Morpholino)-2-butynyl cyclohexanecarboxylate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of water soluble 4-amino-2-butynyl esters having anticancer activity)

RN 35956-47-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)

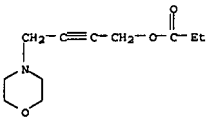
RN 35956-48-0 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



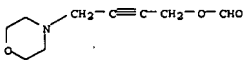
RN 54757-85-6 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, benzoate (ester) (9CI) (CA INDEX NAME)



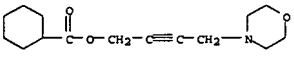
RN 106087-86-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, propanoate (ester) (9CI) (CA INDEX NAME)



RN 866549-52-2 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, formate (ester) (9CI) (CA INDEX NAME)



RN 866549-56-6 CAPLUS
CN Cyclohexanecarboxylic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

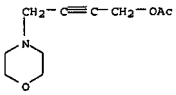
L4 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:561937 CAPLUS
DOCUMENT NUMBER: 143:221810
TITLE: Virtual Screen for Ligands of Orphan G Protein-Coupled Receptors
AUTHOR(S): Bock, Joel R.; Gough, David A.
CORPORATE SOURCE: Department of Bioengineering, University of California San Diego, La Jolla, CA, 92093-0412, USA
SOURCE: Journal of Chemical Information and Modeling (2005), 45(5), 1402-1414
CODEN: JCISD8; ISSN: 1549-9596
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper describes a virtual screening methodol. that generates a ranked list of high-binding small mol. ligands for orphan G protein-coupled receptors (oGPCRs), circumventing the requirement for receptor three-dimensional structure determination Features representing the receptor are based only on physicochem. properties of primary amino acid sequence, and ligand features use the two-dimensional atomic connection topol. and atomic properties. An exptl. screen comprised nearly 2 million hypothetical oGPCR-ligand complexes, from which it was observed that the top 1.96% predicted affinity scores corresponded to "highly active" ligands against orphan receptors. Results representing predicted high-scoring novel ligands for many oGPCRs are presented here. Validation of the method was carried out in several ways: (1) A random permutation of the structure-activity relation of the training data was carried out; by comparing test statistic values of the randomized and non-shuffled data, we conclude that the value obtained with non-shuffled data is unlikely to have been encountered by chance. (2) Biol. activities linked to the compds. with high cross-target binding affinity were analyzed using computed log-odds from a structure-based program. This information was correlated with literature citations where GPCR-related pathways or processes were linked to the bioactivity in question. (3) Anecdotal, out-of-sample predictions for nicotinic targets and known ligands were performed, with good accuracy in the low-to-high "active" binding range. (4) An out-of-sample consistency check using the com. antipsychotic drug olanzapine produced "active" to "highly-active" predicted affinities for all oGPCRs in our study, an observation that is consistent with documented findings of cross-target affinity of this compound for many different GPCRs. It is suggested that this virtual screening approach may be used in support of the functional characterization of oGPCRs by identifying potential cognate ligands. Ultimately, this approach may have implications for pharmaceutical therapies to modulate the activity of faulty or disease-related cellular signaling pathways. In addition to application to cell surface receptors, this approach is a generalized strategy for discovery of small mols. that may bind intracellular enzymes and involve protein-protein interactions.

IT 35956-47-9
RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)
(virtual screen for ligands of orphan G protein-coupled receptors)

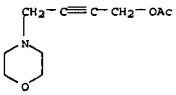
RN 35956-47-9 CAPLUS

L4 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 108 THERE ARE 108 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
G-protein coupled receptor-ligand interactions and other biomol. interactions for drug design uses)
RN 35956-47-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:219996 CAPLUS
DOCUMENT NUMBER: 142:294328
TITLE: Trainable system for predicting G-protein coupled receptor-ligand interactions and other biomolecular interactions for drug design uses
INVENTOR(S): Gough, David A.; Bock, Joel R.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 21 pp., Cont.-in-part of U.S. Ser. No. 993,272.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005053999	A1	20050310	US 2004-973576	20041026
US 2002090631	A1	20020711	US 2001-993272	20011114
WO 2006057763	A2	20060601	WO 2005-US38693	20051025

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.:	US 2000-248258P	P 20001114
	US 2001-993272	A2 20011114
	US 2004-973576	A 20041026

AB The invention is a teachable system and method for predicting the interactions of proteins with other proteins, nucleic acids and small mols. A database containing protein sequences and information regarding protein interactions is used to "teach" the machine. Proteins with unknown interactions are compared by the machine to proteins in the database. Homologs of proteins known to interact in the database are predicted to interact. The invention is used for anal. of protein-protein interactions and protein-nucleic acid interactions, for prediction of protein epitopes, and for whole proteome interaction anal. Virtual screen for ligands of orphan G-protein coupled receptors is provided. The method of the invention can be used in drug design.
IT 35956-47-9
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(predicted high-affinity ligands; trainable system for predicting

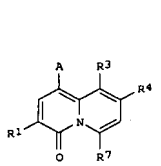
L4 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:407803 CAPLUS
DOCUMENT NUMBER: 129:81674
TITLE: Preparation and use of bi- and tricyclic pyridone derivatives against Alzheimer's disease
INVENTOR(S): Huber, Trottmann Gerda; Jakob-Roetne, Roland; Kolczewski, Sabine; Norcross, Roger David; Woltering, Thomas Johannes
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825930	A2	19980618	WO 1997-EP6865	19971209
WO 9825930	A3	19980813		

W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, GM, SZ, BE, FR, GR, IE, IT, MC, NL, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

US 5869500	A	19990209	US 1997-976541	19971124
AU 9857552	A	19980703	AU 1998-57552	19971209
US 6030984	A	20000229	US 1998-161853	19980928
PRIORITY APPLN. INFO.:			EP 1996-120050	A 19961213
			EP 1997-115614	A 19970909
			US 1997-976541	A3 19971124
			WO 1997-EP6865	W 19971209

OTHER SOURCE(S): MARPAT 129:81674
GI



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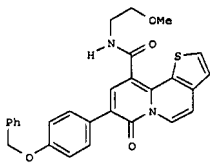


II

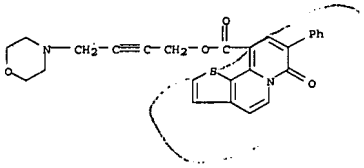
L4 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB The title compds. [I; A = H, C(O)R2, 3-cyclopropyl-1,2,4-oxadiazol-5-yl; R1 = (un)substituted Ph; R2 = lower alkyl, Q1-R5; Q1 = O, NR6; R3, R4 = H; R3R4 = SCH:CH; CH:CHS; CH:CHCH:CH, etc.; R5 = H, lower alkyl, lower alkenyl, etc.; R6 = H, lower alkyl, Ph, etc.], useful for the prophylaxis or treatment of illnesses which are connected with an inhibition of β-amyloid peptide activity, especially for the treatment of Alzheimer's disease, were prepared Thus, treatment of 8-(4-benzyloxyphenyl)-7-oxo-7H-thieno[2,3-a]quinolizine-10-carboxylaic acid (preparation described) with SOCl2 in PhMe followed by reaction of the intermediate with 2-methoxyethylamine in dioxane afforded 74% the title compound II which showed IC50 of 22 μM against Aβ production (measured using sandwich-ELISA in HEK cells).

IT 209333-45-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of bi- and tricyclic pyridone deriva. against Alzheimer's disease)

RN 209333-45-9 CAPLUS

CN 7H-Thieno[2,3-a]quinolizine-10-carboxylic acid, 7-oxo-8-phenyl-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN

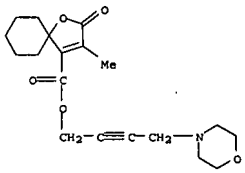
ACCESSION NUMBER: 1991:74807 CAPLUS
DOCUMENT NUMBER: 114:74807
TITLE: Synthesis of acetylenic spirobutenolide derivatives and evaluation of their growth inhibitory effect on cells in culture
AUTHOR(S): Bador, P.; Chantepie, J.; Paris, J.; Quash, G.
CORPORATE SOURCE: Lab. Chim. Ther., Fac. Pharm., Lyon, F-69373, Fr.
SOURCE: Arzneimittel-Forschung (1990), 40(10), 1135-9
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Acetylenic spirobutenolide amides and esters and their Mannich bases were synthesized to evaluate their growth inhibitory effect. The biol. tests used both normal and transformed cells and they show the selectivity of the prepared compds. The ester derivs. presented the best selectivity comparable to that of daunorubicin.

IT 131967-24-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and growth inhibitory activity of, as acetylenic spirobutenolide derivative)

RN 131967-24-3 CAPLUS

CN 1-Oxaspiro[4.5]dec-3-ene-4-carboxylic acid, 3-methyl-2-oxo-, 4-(4-morpholinyl)-2-butynyl ester, hydrochloride (9CI) (CA INDEX NAME)



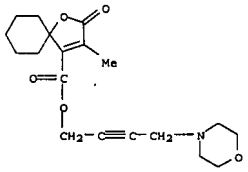
● HCl

IT 131926-46-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antitumor acetylenic spirobutenolide derivs.)

RN 131926-46-0 CAPLUS

CN 1-Oxaspiro[4.5]dec-3-ene-4-carboxylic acid, 3-methyl-2-oxo-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1990:571476 CAPLUS
DOCUMENT NUMBER: 113:171476
TITLE: Preparation of butynylamine derivatives for treatment of pollakiuria and like diseases
INVENTOR(S): Kimura, Kiyoshi; Kise, Masahiro; Morita, Iwao
PATENT ASSIGNEE(S): Nippon Shinyaku Co., Ltd., Japan
SOURCE: Brit. UK Pat. Appl., 40 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2222828	A	19900321	GB 1989-20766	19890913
GB 2222828	B	19920429		
IL 91377	A	19960912	IL 1989-91377	19890822
CN 1041582	A	19900425	CN 1989-106930	19890830
CN 1038410	B	19980520		
EP 359311	A2	19900321	EP 1989-202235	19890905
EP 359311	A3	19910703		
EP 359311	B1	19970115		
R: DE, IT, NL, SE				
ES 2016060	A6	19901001	ES 1989-3097	19890912
KR 154325	B1	19981201	KR 1989-13217	19890912
JP 02218651	A	19900831	JP 1989-238272	19890913
JP 06069996	B	19940907		
HU 58045	A2	19920128	HU 1989-4825	19890913
CH 680440	A5	19920831	CH 1989-3344	19890913
CA 1317943	C	19930518	CA 1989-611310	19890913
FR 2639044	A1	19900518	FR 1989-12032	19890914
FR 2639044	B1	19930806		
US 5036098	A	19910730	US 1989-407228	19890914
BE 1003256	A5	19920211	BE 1989-977	19890914
US 5036098	B1	19931102	US 1992-900028826	19920831

PRIORITY APPLN. INFO.: JP 1988-231272 A 19880914
US 1989-407228 A 19890914

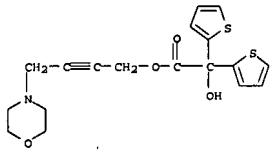
OTHER SOURCE(S): CASREACT 113:171476; MARPAT 113:171476

AB The title derivs. of the R1R2C(OH)COACR3R4C.tplbond.CCH2NR5R6 (R1, R2 = cycloalkyl, Ph, or 2-thienyl; R3, R4 = H, alkyl, or together with the adjacent C form a cycloalkyl; R5, R6 = H, alkyl; or together with the N form a cyclic amino; A = O or NR where R = H or alkyl), and their pharmacol. acceptable salts, are prepared The derivs. show anticholinergic and Ca2+ antagonism. Thus, to a heated mixture containing 1,1-dimethyl-2-propynyl α-cyclohexyl-α-phenylglycolate, paraformaldehyde, and CuCl in dioxane was added Et2N to give 4-diethylamino-1,1-dimethyl-2-butynyl α-cyclohexyl-α-phenylglycolate (I), which was isolated as the HCl salt. I·HCl showed PA2 values for anticholinergic action and Ca2+ antagonism upon detrusor muscles of excised rabbit bladder of 7.33 and 6.72, resp.

IT 129927-39-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as anticholinergic and calcium antagonist)

RN 129927-39-5 CAPLUS

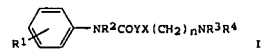
L4 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Thiopheneacetic acid, α-hydroxy-α-2-thienyl-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



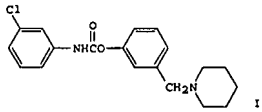
L4 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:57493 CAPLUS
DOCUMENT NUMBER: 110:57493
TITLE: Heterocyclylalkylphenyl N-phenylcarbamate derivatives as acetylcholinesterase inhibitors, their preparation, and formulations containing them
INVENTOR(S): Tamura, Toshiya; Tsukamoto, Shinichi; Usuda, Shinji; Harada, Masatomi
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 40 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63170356	A	19880714	JP 1986-311852	19861230
PRIORITY APPLN. INFO.:			JP 1986-311852	19861230

OTHER SOURCE(S): MARPAT 110:57493
GI



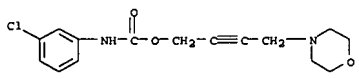
I



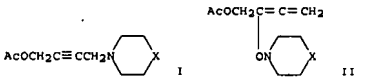
II

AB The title compds. I [R1 = H, halo, lower alkoxy, OH, etc.; R2 = H, lower alkyl; NR3R4 = (substituted) heterocyclyl which may be fused to a benzene ring; n = 1-5; Y = O, S, imino; X = CH2CH:CH, CH2C.tplbond.C, etc.], useful as acetylcholinesterase inhibitors, were prepared A mixture of m-(piperidinomethyl)phenol and m-ClC6H4NCO in C6H6 was refluxed for 2 h to give carbamate II. II in vitro exhibited an IC50 of 0.12 μM against acetylcholinesterase.
IT 118511-48-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as acetylcholinesterase inhibitor)
RN 118511-48-1 CAPLUS
CN Carbamic acid, (3-chlorophenyl)-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)

L4 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

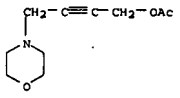


L4 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:406012 CAPLUS
DOCUMENT NUMBER: 109:6012
TITLE: Carbon-13 NMR study of some acetylenic amines, their N-oxides and their rearrangement products
AUTHOR(S): Al-Rawi, Jasim M. A.; Khuthier, Abdul-Hussain; Abachi, Faris T.
CORPORATE SOURCE: Coll. Sci., Univ. Mosul, Mosul, Iraq
SOURCE: Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1987), 43A(9), 1121-3
CODEN: SAMCAS; ISSN: 0584-8539
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:6012
GI



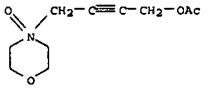
I II

AB The 13C NMR spectra of acetylenic amines I (X = a bond, CH2, CHMe, O, CH2CH2, etc.) and some of their N-oxides were analyzed. Thermal rearrangement of the oxides gave allenes (II).
IT 35956-47-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, carbon-13 NMR and oxidation of)
RN 35956-47-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)



IT 114906-22-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, carbon-13 NMR and rearrangement of)
RN 114906-22-8 CAPLUS
CN 2-Butyn-1-ol, 4-(4-oxido-4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)

L4 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L4 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 144-62-7
CMF C2 H2 O4

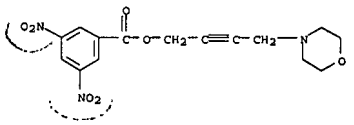
L4 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:515227 CAPLUS
DOCUMENT NUMBER: 107:115227
TITLE: Acetylenic amines of potential pharmacological value
AUTHOR(S): Abachi, F. T.; Yousif, W. H.; Al-Rawi, M. M.; Khodr, A. M.; Khuthier, A. H.
CORPORATE SOURCE: Coll. Vet. Med., Univ. Mosul, Mosul, Iraq
SOURCE: Journal of the Iraqi Chemical Society (1986), 11(1), 105-14
CODEN: JICSDK; ISSN: 0379-8321
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:115227

AB Amines R1CH2C.tplbond.CCH2NR2 [R1 = MeO, 3,5-(O2N)2C6H3CO2; NR2 = piperidino, morpholino, 4-formyl-1-piperazinyl], which showed mydriatic activity and its usefulness in the treatment of Parkinsonism, were prepared by the Mannich reaction.

IT 110197-02-9P 110197-03-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and pharmacol. activity of)

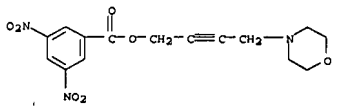
RN 110197-02-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, 3,5-dinitrobenzoate (ester) (9CI) (CA INDEX NAME)



RN 110197-03-0 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, 3,5-dinitrobenzoate (ester), ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

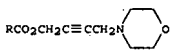
CM 1

CRN 110197-02-9
CMF C15 H15 N3 O7



L4 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1987:32952 CAPLUS
DOCUMENT NUMBER: 106:32952
TITLE: Synthesis and properties of acetylenic amino esters of some aliphatic acids
AUTHOR(S): Ergashev, M. S.; Kasymova, S. S.; Kulakhmatova, M. A.
CORPORATE SOURCE: Tashk. Gos. Univ., Tashkent, USSR
SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya (1986), 29(1), 39-41
CODEN: IVUKAR; ISSN: 0579-2991
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 106:32952
GI

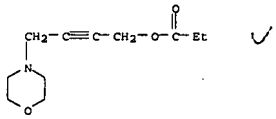


I

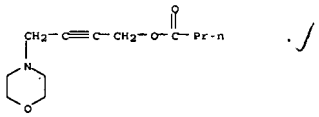
AB Morpholinobutynyl alkanoates I (R = C2-C9 n-alkyl) were prepared in 72.4-83.2% yields by Mannich reactions of morpholine and paraformaldehyde with RCO2CH2C.tplbond.CH in dioxane containing CuCl.

IT 106087-86-9P 106087-87-0P 106087-88-1P
106087-89-2P 106087-90-5P 106087-91-6P
106087-92-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

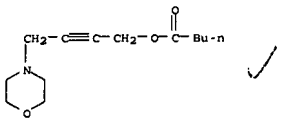
RN 106087-86-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, propanoate (ester) (9CI) (CA INDEX NAME)



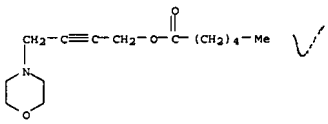
RN 106087-87-0 CAPLUS
CN Butanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



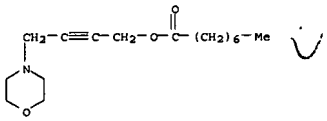
L4 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 106087-88-1 CAPLUS
CN Pentanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



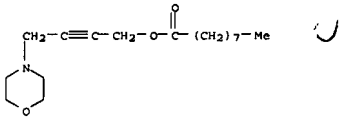
RN 106087-89-2 CAPLUS
CN Hexanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



RN 106087-90-5 CAPLUS
CN Octanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)

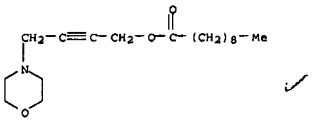


RN 106087-91-6 CAPLUS
CN Nonanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



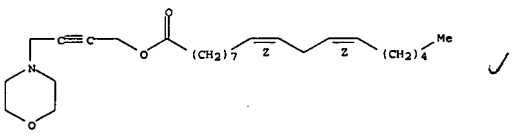
L4 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 106087-92-7 CAPLUS
CN Decanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



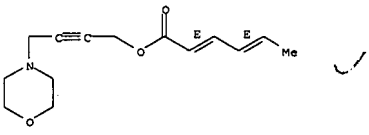
L4 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:27650 CAPLUS
DOCUMENT NUMBER: 106:27650
TITLE: Synthesis and hypocholesterolemic activity of aminobutynyl linoleates
AUTHOR(S): Ergashev, M. S.; Makhsumov, A. G.; Khadzhiev, A. K.
CORPORATE SOURCE: Med. Inst., Tashkent, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1986), 20(9), 1050-1
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Me(CH2)4CH:CHCH2CH:CH(CH2)7CO2CH2C.tplbond.CCH2NR2 (I, R = Et or CH2Ph or NR2 = piperidinyl or morpholinyl) were prepared from propargyl linoleate [106059-79-4], CH2O and the appropriate amine. In studies in rabbits with exptl. atherosclerosis and hypercholesterolemia, I (NR2 = morpholino) [106059-82-9] and I (R = CH2Ph) [106059-83-0] were more active as hypocholesterolemics than were the other 2 compds. All were more effective than the hypocholesterolemic Arakhides.
IT 106059-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hypocholesterolemic activity of)
RN 106059-82-9 CAPLUS
CN 9,12-Octadecadienoic acid (9Z,12Z)-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



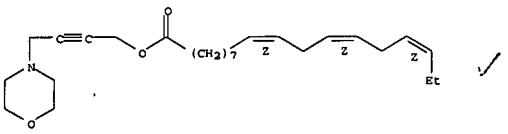
L4 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:4504 CAPLUS
DOCUMENT NUMBER: 106:4504
TITLE: Amino ester acetylene derivatives of sorbic acid
AUTHOR(S): Makhsumov, A. G.; Tadzhibaev, U.; Ergashev, M. S.
CORPORATE SOURCE: Tashk. Gos. Med. Inst., Tashkent, USSR
SOURCE: Uzbekskii Khimicheskii Zhurnal (1985), (5), 63-5
CODEN: UZKZAC; ISSN: 0042-1707
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Mannich reaction of propargyl sorbate with R2NH (R = hexyl, octyl, PhCH2; R2N = morpholino, anabasino, cytisino) and paraform in dioxane containing Cu(OAc)2 at 100-105° gave 6 corresponding Me(CH:CH)2CO2CH2C.tplbond.CCH2NR2 in 76.1-92.1% yield.
IT 105566-28-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by Mannich reaction of propargyl sorbate)
RN 105566-28-7 CAPLUS
CN 2,4-Hexadienoic acid, 4-(4-morpholinyl)-2-butynyl ester, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

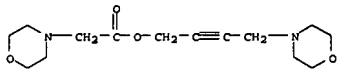


L4 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:406587 CAPLUS
DOCUMENT NUMBER: 101:6587
TITLE: Hypolipidemic activity of derivatives of propargyl esters of linolenic acids
AUTHOR(S): Makhsumov, A. G.; Khadzhiev, A. K.; Gul'mirzaeva, I. K.; Khadzhiev, K. Kh.; Ergashev, M. S.; Madikhanov, N.
CORPORATE SOURCE: USSR
SOURCE: Piziol. Aktiv. Veshchestva (1983), (15), 62-6
From: Ref. Zh., Khim. 1984, Abstr. No. 3Zh107
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 101:6587
AB Title only translated.
IT 90430-69-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and hypolipidemic activity of)
RN 90430-69-6 CAPLUS
CN 9,12,15-Octadecatrienoic acid, 4-(4-morpholinyl)-2-butynyl ester, (Z,Z,Z)-
(9CI) (CA INDEX NAME)

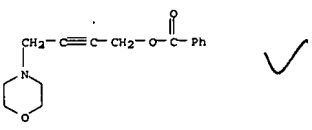
Double bond geometry as shown.



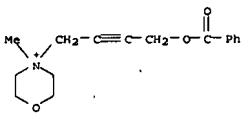
L4 ANSWER 14 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1979:125487 CAPLUS
DOCUMENT NUMBER: 90:125487
TITLE: Study of the inhibiting properties of 1-chloro-2-oxo-3-oxa-5-hexyne and its amino derivatives in the acid corrosion of metals
AUTHOR(S): Tsalikova, Z. M.; Karaev, S. F.; Shikhiev, I. A.; Asadullaev, A. F.
CORPORATE SOURCE: Azerb. Inst. Nefti Khim., Baku, USSR
SOURCE: Azerbaidzhanskii Khimicheskii Zhurnal (1978), (3), 83-5
CODEN: AZKZAU; ISSN: 0005-2531
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The inhibiting effects of RCH2CO2C.tplbond.CCH2R1 (I; R = H, Cl, Et2N, Bu2N, piperidino, or morpholino; R1 = H, Et2N, Bu2N, piperidino, or morpholino) on the corrosion of St. 3 [39296-41-8] in 4 N HCl at 60° were studied. In general, the corrosion inhibiting effect was decreased, compared to I (R = Cl, R1 = H) [627-09-8], with introduction of an amino substituent in the acetate moiety; i.e., I (R = Et2N, piperidino, or morpholino, R1 = H); however, the greatest inhibiting effect was exhibited by I (R = Bu2N, R1 = H) [54480-21-6]. Introduction of 2 amino substituents decreased the inhibiting effect by a factor of .apprx.2.
IT 54928-26-6
RL: USES (Uses)
(corrosion inhibition by, of steel in hydrochloric acid solution)
RN 54928-26-6 CAPLUS
CN 4-Morpholineacetic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:409070 CAPLUS
DOCUMENT NUMBER: 83:9070
TITLE: Synthesis of γ-substituted propargyl alcohols, their ethers and esters
AUTHOR(S): Kruglikova, R. I.; Berestevich, B. K.; Babaeva, L. G.; Unkovskii, B. V.
CORPORATE SOURCE: Mosk. Inst. Tonkoi Khim. Tekhnol. im. Lomonosova, Moscow, USSR
SOURCE: Izvestiya Vysshikh Uchebnykh Zavedenii, Khimiya i Khimicheskaya Tekhnologiya (1974), 17(12), 1824-7
CODEN: IVUKAR; ISSN: 0579-2991
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB RC.tplbond.CCH2OH (R = Me, MeOCH2, CH2:CH, Ph, Me2NCH2, Me2C(OH), 1-hydroxycyclohexyl, PhCH(OH)) were prepared in 38-59% yield. E.g., H2C:CH2C.tplbond.CCH2OH was prepared by treatment of HC.tplbond.CCH:CH2 with EtMgBr, followed by HCHO. R1C.tplbond.CCH2OMe [R1 = H, Me, MeOCH2, Ph, Me2NCH2, MeCO2CH2, ClCH2, BrCH2, MeC(OH)] were prepared in 39-85% yield, usually by methylation of the resp. alcs. RC.tplbond.CCH2O2CC6H4NO2-p (R = H, Me, MeOCH2, Ph, Me2NCH2, Br) and RC.tplbond.CCH2O2CPh (R = H, Me, MeOCH2, CH2:CH, Ph, 1-hydroxycyclohexyl, Me2NCH2, Et2NCH2, piperidinomethyl, morpholinomethyl) were prepared by standard methods.
IT 54757-85-6P 54757-94-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54757-85-6 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, benzoate (ester) (9CI) (CA INDEX NAME)



RN 54757-94-7 CAPLUS
CN Morpholinium, 4-[4-(benzoyloxy)-2-butynyl]-4-methyl-, iodide (9CI) (CA INDEX NAME)

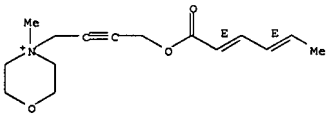


● I⁻

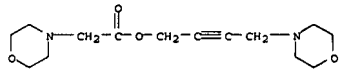
L4 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:149868 CAPLUS
DOCUMENT NUMBER: 82:149868
TITLE: Physiological activity of new aminoacetylenic sorbic acid esters
AUTHOR(S): Abdullaev, Sh. U.; Makhsumov, A. G.; Usmanov, M.
CORPORATE SOURCE: Tashk. Gos. Univ., Tashkent, USSR
SOURCE: Dokl. Vses. Konf. Khim. Atsetilena, 4th (1972), Meeting Date 1972, Volume 1, 500-3. Editor(s): Azerbaev, I. N. Akad. Nauk Kaz. SSR, Inst. Khim. Nauk: Alma-Ata, USSR.
CODEN: 30AKA7
DOCUMENT TYPE: Conference
LANGUAGE: Russian
AB Iodomethylates of 6 sorbic acid aminoacetylenic esters showed bactericidal activity against 7 pyrogenic and intestinal bacterial species. Even the most active of these compds., sorbic acid 4-(N-3-methylpiperidinobut-2-ynyl) ester iodomethylate [54951-08-5], was somewhat less effective than several commonly used antibiotics.
IT 54951-10-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal activity of)
RN 54951-10-9 CAPLUS
CN Morpholinium, 4-methyl-4-[4-[(1-oxo-2,4-hexadienyl)oxy]-2-butynyl]-, iodide, (E,E)- (9CI) (CA INDEX NAME)

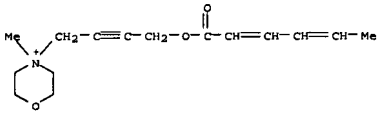
Double bond geometry as shown.



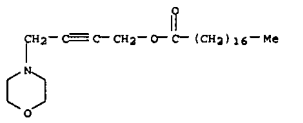
L4 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1975:124676 CAPLUS
DOCUMENT NUMBER: 82:124676
TITLE: Reaction of 2-propyn-1-ol chloroacetate with amines
AUTHOR(S): Karaev, S. F.; Tsalikova, Z. M.; Shikhiev, I. A.
CORPORATE SOURCE: Azerb. Inst. Nefti Khim. im. Azizbekova, Baku, USSR
SOURCE: Azerbaidzhanskii Khimicheskii Zhurnal (1974), (4), 30-3
CODEN: AZKZAU; ISSN: 0005-2531
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The reaction of ClCH2COCl with HOCH2C.tplbond.CH gave HC.tplbond.CCH2O2CCH2Cl, which was aminated with HNR2 to give HC.tplbond.CCH2O2CCH2NR2 (I, NR2 = NEt2, NBu2, piperidino, morpholino). II were aminomethylated with paraformaldehyde in HNR12 to give R12NCH2C.tplbond.CCH2O2CCH2NR2 (R12N, R2N given): Et2N, Et2N; bu2N, Bu2N; piperidino, piperidino; morpholino, morpholino; piperidino, Et2N.
IT 54928-26-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54928-26-6 CAPLUS
CN 4-Morpholineacetic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



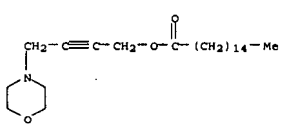
L4 ANSWER 18 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:536947 CAPLUS
DOCUMENT NUMBER: 79:136947
TITLE: Sorbates of acetylenic amino alcohols
AUTHOR(S): Makhsumov, A. G.; Abdullaev, Sh. U.
CORPORATE SOURCE: USSR
SOURCE: Khim. Atsetilena Tekhnol. Karbida Kal'tsiya (1972) 96-7
From: Ref. Zh., Khim. 1973, Abstr. No. 9Zh368
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Paraformaldehyde (0.15 mole), 0.12 mole piperidine, 0.1 mole propargyl sorbate, CuCl, and dioxane was heated 7 hr at 94-6°, and the product converted into the methiodide to give 90% MeCH:CHCH:CHCO2CH2C.tplbond.CCH2R.MeI (I) (R = piperidino). Other I prepared were (R and % yield given): 2-methylpiperidino, 87.5; 3-methylpiperidino, 88.2; 4-methylpiperidino, 87; 5-ethyl-2-methylpiperidino, 75.6; morpholino, 91.3; 2-(3-pyridyl)piperidino, 85; and hexahydroazepino, 85.
IT 50669-11-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 50669-11-9 CAPLUS
CN Morpholinium, 4-methyl-4-[4-[(1-oxo-2,4-hexadienyl)oxy]-2-butynyl]-, iodide (9CI) (CA INDEX NAME)



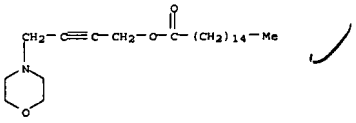
L4 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:71357 CAPLUS
DOCUMENT NUMBER: 78:71357
TITLE: Synthesis and properties of acetylenic amino esters of palmitic and stearic acids
AUTHOR(S): Abdurakhimov, A.; Maksumov, A. G.; Il'khamdzhanov, P.
CORPORATE SOURCE: USSR
SOURCE: Tr. Inst. Khim. Nefti Prirod. Solei, Akad. Nauk Kaz. SSR (1971), No. 3, 145-9
From: Ref. Zh., Khim. 1972, Abstr. No. 4Zh164
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Mannich reaction of propargyl esters of palmitic and stearic acids in dioxane with Cu2I2 [better than Cu(AcO)2, Cu2Cl2, CuCl2, Cu2Br2, or CuBr2] as catalyst gave Me(CH2)nCO2CH2C.tplbond.CCH2Z (Z and % yield for n = 14 and n = 16 given): morpholino, 79, 79.6; piperidino, 79.6, 82.8; 2-methylpiperidino, 66.3, 74.9; 3-methylpiperidino, 70, 77.9; 4-methylpiperidino, 78.8, 80.1; 5-ethyl-2-methylpiperidino, 66.1, 69.8; 2-(3-pyridyl)piperidino, 78.9, 79.4; Me2N, 74.4, 67.9; Et2N, 70.8, 82.2; Bu2N, 79.3, 82.1; and Bz2N (sic), 86.7, 87.4.
IT 29237-96-5P 38022-01-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29237-96-5 CAPLUS
CN Octadecanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



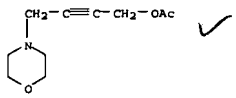
RN 38022-01-4 CAPLUS
CN Hexadecanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



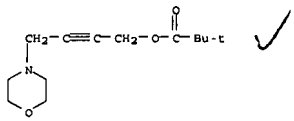
L4 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:526576 CAPLUS
DOCUMENT NUMBER: 77:126576
ORIGINAL REFERENCE NO.: 77:20853a,20856a
TITLE: Condensation of propargyl palmitate with amines
AUTHOR(S): Abdurakhimov, A.; Makhsumov, A. G.; Safaev, A. S.; Il'khamdzhanov, P.
CORPORATE SOURCE: USSR
SOURCE: Tr. Tashkent. Politekh. Inst. (1970), No. 64, 29-32
From: Ref. Zh., Khim. 1971, Abstr. No. 22Zh230
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB The maximum yield is obtained in the title reaction if HCHO is used, rather than (HCHO)x, and Cu(OAc)2 is used as catalyst. Thus, 0.015 mole 40% HCHO, 0.01 mole piperidine, 0.01 mole Me(CH2)14CO2CH2C.tplbond.CH, 40 ml dioxane, and 0.15 g Cu(OAc)2 was heated 6 hr at 96-8° to give 83% Me(CH2)14CO2CH2C.tplbond.CCH2R (R = piperidino). Similarly prepared was 82.8% morpholino analog.
IT 38022-01-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 38022-01-4 CAPLUS
CN Hexadecanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



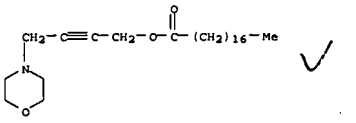
L4 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:108230 CAPLUS
DOCUMENT NUMBER: 76:108230
ORIGINAL REFERENCE NO.: 76:17421a,17424a
TITLE: 4-Amino-2-buten-1-ol esters
AUTHOR(S): Willette, Robert E.; Driscoll, Richard C.
CORPORATE SOURCE: Sch. Pharm., Univ. Connecticut, Storrs, CT, USA
SOURCE: Journal of Medicinal Chemistry (1972), 15(1), 110-12
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Trans-4-amino-2-butene-1-ol esters, R2NCH2CH:CHCH2O2CR1, where R2N = Me2N or morpholino and R1 = Me or iso-Pr, were prepared by condensation of the desired amine with 4-chloro-2-butyn-1-ol, followed by LiAlH4 reduction and esterification. The corresponding cis isomers were prepared by esterification of the aminobutynol followed by catalytic reduction with H2 and Pd/C. None of these compds. (100mg/kg/week, 8 weeks) showed any hepatotoxicity in mice.
IT 35956-47-9P 35956-48-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 35956-47-9 CAPLUS
CN 2-Butyn-1-ol, 4-(4-morpholinyl)-, acetate (ester) (9CI) (CA INDEX NAME)



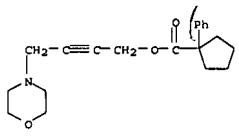
RN 35956-48-0 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:487375 CAPLUS
DOCUMENT NUMBER: 73:87375
ORIGINAL REFERENCE NO.: 73:14280h,14281a
TITLE: Derivatives of stearic acid aminoester acetylenes
AUTHOR(S): Il'khamdzhanov, P.; Makhsumov, A. G.; Abaurakhimov, A.
CORPORATE SOURCE: USSR
SOURCE: Zhurnal Prikladnoi Khimii (Sankt-Peterburg, Russian Federation) (1970), 43(6), 1414-15
CODEN: ZPKHAB; ISSN: 0044-4618
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Me(CH2)16CO2CH2C.tplbond.CCH2NR2 [NR2 = morpholino, piperidino, NPh2, N(CH2Ph)2] were synthesized in 75-88% yield from formalin, Me(CH2)16CO2CH2C.tplbond.CH, and the corresponding amine in dioxane by the use of Cu(OAc)2.
IT 29237-96-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 29237-96-5 CAPLUS
CN Octadecanoic acid, 4-(4-morpholinyl)-2-butynyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 23 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:447998 CAPLUS
DOCUMENT NUMBER: 71:47998
ORIGINAL REFERENCE NO.: 71:8815a,8818a
TITLE: Acetylene compounds of potential pharmacological value. XII. Central and peripheral anticholinergic activity of tertiaryaminoalkynyl esters of some carboxylic acids
AUTHOR(S): Dahlbom, Richard; Erbing, Birgitta; Olsson, Kerstin; George, Robert; Jenden, Donald J.
CORPORATE SOURCE: Farm. Fak., Stockholm, Swed.
SOURCE: Acta Pharmaceutica Suecica (1969), 6(3), 349-58
CODEN: APSXAS; ISSN: 0001-6675
DOCUMENT TYPE: Journal
LANGUAGE: English
AB tert-Aminoalkynyl esters of 1-phenylcyclopentanecarboxylic acid, 1-phenyl-cyclohexanecarboxylic acid, and benzilic acid were more active than the esters of diphenylacetic acid and phenothiazine-10-carboxylic acid when tested for antagonist activity toward acetylcholine on isolated guinea pig ileum and for mydriatic activity in intact mice. Generally the esters of benzilic acid appeared to have the highest potency. The most effective of these compds. was about half as active as atropine in blocking the central effects of oxotremorine and its effect on contractions of the guinea pig ileum induced by acetylcholine was .apprx.14% that of atropine.
IT 24642-37-3
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacology of)
RN 24642-37-3 CAPLUS
CN Cyclopentanecarboxylic acid, 1-phenyl-, 4-morpholino-2-butynyl ester (8CI)
(CA INDEX NAME)

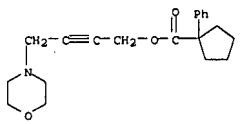


L4 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1968:49456 CAPLUS
DOCUMENT NUMBER: 68:49456
ORIGINAL REFERENCE NO.: 68:9563a,9566a
TITLE: 4-Dialkylamino-2-butynyl-1-phenylcycloalkanecarboxylates
INVENTOR(S): Dahlbom, Richard
PATENT ASSIGNEE(S): Aktiebolag Astra
SOURCE: U.S., 2 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3317526		19670502	US	19640716

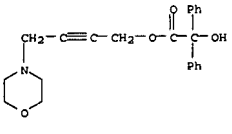
GI For diagram(s), see printed CA Issue.
AB The title compds. exhibit tremorolytic action with a min. of side-effects, and thus are effective in therapy of Parkinson's disease. They are made preferably via the Mannich reaction, but alternative routes are possible. Thus, a mixture of 35 g. 1-phenyl-1-cyclopentanecarbonyl chloride (I) and 10 g. propargyl alc. was refluxed 15 min. and fractionated in vacuo to give propargyl 1-phenyl-1-cyclopentanecarboxylate (II), b0.3 107-8°. A solution of 10 g. II, 3.4 g. pyrrolidine, 1.6 g. (CH2O)n, and 0.15 g. CuCl in 30 cc. dioxane was refluxed 10 min., treated with 150 cc. H2O, extracted with Et2O (extract discarded), and alkalized with 5N NH4OH. The precipitated amino ester was taken up in Et2O, the solution dried, and the HCl salt precipitated with HCl in Et2O to give 4-pyrrolidino-2 - butynyl 1 - phenyl - 1 - cyclopentanecarboxylate (III).HCl, m. 105-7° (2:1 EtOH-Et2O). Similarly prepared were: 4-diethylamino-2-butynyl 1-phenyl-1-cyclopentanecarboxylate-HCl (IV), m. 93-4°; 4-diethylamino-2-butynyl 1-phenyl-1-cyclohexanecarboxylate-HCl, m. 126-8°; and 4-piperidino-2-butynyl 1-phenyl-1-cyclopentanecarboxylate-HCl, m. 124-6°. A solution of 11.5 g. I, 7 g. 4-diethylamino-2-butyn-1-ol (V), and 6 g. NEt3 in 75 cc. C6H6 was refluxed 2 hrs., cooled, and filtered, the filtrate worked up, and the product treated with HCl in Et2O to give IV. Similarly prepared were: 4-pyrrolidino-2-butynyl 1-phenyl-1-cyclohexanecarboxylate-HCl, m. 127-9°; 4-morpholino-2-butynyl 1-phenyl-1-cyclopentanecarboxylate-HCl, m. 123-5°. To 7 g. V were added 0.5 g. Na and 2.5 g. methyl 1-phenyl-1-cyclopentanecarboxylate (VI) and the mixture heated 3 hrs. at 50°/10 mm., thus removing MeOH as formed. After dilution with 100 cc. H2O and acidification to pH 5, unchanged VI was extracted with 50 cc. Et2O, the solution alkalized and extracted with Et2O, and IV isolated as above.
IT 17781-98-5P
RL: SPN (Synthetic preparation); PREP (Preparation)

L4 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. of)
RN 17781-98-5 CAPLUS
CN Cyclopentanecarboxylic acid, 1-phenyl-, 4-morpholino-2-butynyl ester hydrochloride (7CI, 8CI) (CA INDEX NAME)

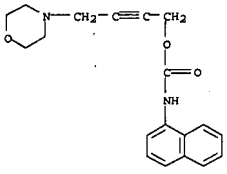


● HCl

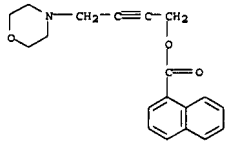
L4 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:18418 CAPLUS
DOCUMENT NUMBER: 66:18418
ORIGINAL REFERENCE NO.: 66:3523a,3526a
TITLE: Mannich reaction with propargyl alcohol
AUTHOR(S): Salvador, Romano L.; Simon, D.
CORPORATE SOURCE: Univ. Montreal, Montreal, Can.
SOURCE: Canadian Journal of Chemistry (1966), 44(21), 2570-5
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 66:18418
GI For diagram(s), see printed CA Issue.
AB A group of aminobutynols (e.g. I. of the type R2NCH2C.tplbond.CCH2OH were prepared from propargyl alc. by the Mannich reaction, using CuSO4 as catalyst, and the probable course of reaction discussed. The effect of pH on the yield in the reaction was studied showing that the reaction should be run in a medium which is acidic enough to form and stabilize the postulated carbenium ion R2NCH2+ but not acidic enough to prevent the formation of Cu acetylide.
IT 14597-23-0P 14597-33-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14597-23-0 CAPLUS
CN Benzilic acid, 4-morpholino-2-butynyl ester (7CI, 8CI) (CA INDEX NAME)



RN 14597-33-2 CAPLUS
CN 1-Naphthalenecarbamic acid, 4-morpholino-2-butynyl ester (8CI) (CA INDEX NAME)



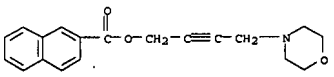
L4 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:471827 CAPLUS
DOCUMENT NUMBER: 63:71827
ORIGINAL REFERENCE NO.: 63:13201d-f
TITLE: Anticholinergic agents-esters of 4-dialkyl(or 4-polymethylene)amino-2-butynols
AUTHOR(S): Majewski, Robert F.; Campbell, Kenneth N.; Dykstra, Stanley; Covington, Robert; Simms, Jack C.
CORPORATE SOURCE: Mead Johnson Res. Center, Evansville, IN
SOURCE: Journal of Medicinal Chemistry (1965), 8(5), 719-20
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4-Dialkyl(or 4-polymethylene)amino-2-butynols (I) were prepared from 4-chloro-2butynol and the corresponding secondary amines (Biel, et al., CA 52, 6335g). Four procedures were used for the preparation of the title esters RCO2CH2C.tplbond.CCH2R' (I): from propargyl alc. analogous to that of Jones (J., et al., CA 42, 8774e); by ester-alc. interchange from a Me ester and the appropriate 4-amino-2-butynol; by esterification of the aminobutynol with an acid chloride; and by ester-ester interchange from e.g. 4-diethylamino-2-butynyl acetate and the Me ester of an appropriate carboxylic acid. The compds. were tested for smooth muscle depressant, local anesthetic, and (or) anticholinergic actions. I.HCl (R = SMe, R' = piperidino) was found to have local anesthetic activity equivalent to lidocaine hydrochloride. I.HCl [R = ZPhCOH (Z = cyclohexyl), R' = NEt2] was found to possess about 10% of the activity of atropine on several types of extravascular smooth muscle plus strong papavarine-like action.
IT 3512-26-3P, 1-Naphthoic acid, 4-morpholino-2-butynyl ester, hydrochloride 3512-28-5P, 2-Naphthoic acid, 4-morpholino-2-butynyl ester, hydrochloride 3512-36-5P, Acetic acid, (methylthio)diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 3512-26-3 CAPLUS
CN 1-Naphthoic acid, 4-morpholino-2-butynyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

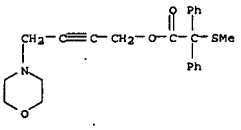
RN 3512-28-5 CAPLUS
CN 2-Naphthoic acid, 4-morpholino-2-butynyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 3512-36-5 CAPLUS
CN Acetic acid, (methylthio)diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)

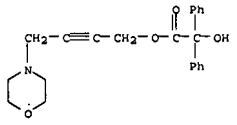


● HCl

L4 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:52495 CAPLUS
DOCUMENT NUMBER: 60:52495
ORIGINAL REFERENCE NO.: 60:9191e-f
TITLE: Acetylene compounds of potential pharmacological value. III. 4-Dialkylamino-2-butynyl esters of benzilic acid
AUTHOR(S): Dahlbom, Richard; Hansson, Birgitta; Mollberg, Rene
CORPORATE SOURCE: Kungl. Farm. Inst., Stockholm
SOURCE: Acta Chemica Scandinavica (1963), 17(8), 2354-6
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 60:52495

AB cf. CA 59, 8729h. The title compds. were prepared by the method of King and Holmes (CA 41, 5121g). Low yields are obtained by trans esterification of Me benzilate with the appropriate 4-dialkylamino-2-butyn-1-ol. The following Ph2CRCO2CH2C.tplbond.CCH2NR12 were prepared (R, R1, derivative, % yield, and m.p. given): Cl, Et, HCl salt, 81, 96-7°; HO, Et, HCl salt, 55, 127-8°, HO, Et, MeBr, 78, 149-50.5°; Cl, (NR12 =) pyrrolidino, HCl salt, 78, 164-5.5°; HO, (NR12 =) pyrrolidino, HCl salt, 86, 137-8° (base m. 110-12°); Cl, (NR12 =) piperidino, HCl salt, 76, 141-2°; HO, (NR12 =) piperidino, HCl salt, 52, 146-7°; HO, (NR12 =) morpholino, HCl salt, 50, 148-9°. The compds. had anticholinergic activity and inhibited tremors due to oxotremorine.

IT 95130-66-8P, Benzilic acid, 4-morpholino-2-butynyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 95130-66-8 CAPLUS
CN Benzilic acid, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L4 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:16636 CAPLUS
DOCUMENT NUMBER: 60:16636
ORIGINAL REFERENCE NO.: 60:2909d-h,2910a-c
TITLE: Aminoacetylenes
PATENT ASSIGNEE(S): Mead Johnson & Co.
SOURCE: 7 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

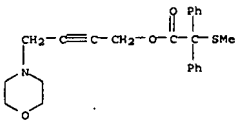
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 940540		19631030	GB 1961-26864	19610725
DE 1216866			DE	
US 3176019		19650330	US 1961-118261	19610620
PRIORITY APPLN. INFO.:			US	19600726

AB A solution of 1.56 g. paraformaldehyde (I) and 2.0 g. Me2NH in 10 ml. dry dioxane was allowed to stand at room temperature 10 min., 10 g. propargyl diphenylacetate in 25 ml. dry dioxane added, the mixture heated on a steam bath 17 hrs. under N and cooled slightly, the unreacted Me2NH removed, 2N HCl added, and the solution washed with Et2O, cooled with crushed ice, and made alkaline with 10% NaOH. The insol. oil was taken up in Et2O, the solution dried (MgSO4) and filtered, dry HCl passed into the solution, and the precipitate filtered off to give 4-dimethyl-2-butynyl diphenylacetate-HCl, m. 180-1.5° (decomposition) (PrOH). Similarly prepared was 4-pyrrolidino-2-butynyl diphenylacetate-HCl, m. 140-2° (EtOAc-PrOH). Diphenylacetyl chloride (15 g.) was slowly added to 10.0 g. 4-piperidino-2-butynol, b1.4 116°, n20D 1.5094 (prepared from 1-chloro-4-hydroxy-2-butyne and piperidine) dissolved in 30 ml. dry pyridine (exothermic reaction), the mixture heated on a steam bath 1 hr., cooled, and poured onto crushed ice-water, the mixture extracted with Et2O, the exts. washed with small portions 2N HCl to remove the residual pyridine, the Et2O solution washed with water and dried over MgSO4, and the product isolated by passing dry HCl into the filtered mixture to give 4-piperidino-2-butynyl diphenylacetate-HCl, m. 155-6.5° (EtOAc). To a solution of 17.2 g. α-chlorodiphenyl-acetyl chloride in 40 ml. dry pyridine was slowly added 7.0 g. 4-pyrrolidino-2-butynol (II), b1.0 98-104°, n20D 1.5055 (prepared from 1-chloro-4-hydroxy-2-butyne and pyrrolidine), and after the vigorous reaction subsided, the mixture poured onto crushed ice-water, the aqueous solution extracted with Et2O, the exts. washed with water and extracted with 2N HCl, and the acidic exts. heated on a steam bath 5 min., cooled, and made alkaline with 10% NaOH, the viscous oil taken up in Et2O, the Et2O solution dried (MgSO4) and filtered, and the Et2O evaporated to give a yellow solid, which was triturated with Et2O to give 4-pyrrolidino-2-butnyl benzilate, m. 108-11.5° (aqueous EtOH) (HCl salt m. 132.5-4.5°)'. Diphenylisobutyryl chloride (18.1 g.) and 21.0 g.

L4 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Et3N were cautiously mixed with 85 ml. anhyd C6H6, 10.1 g. II dissolved in 20 ml. anhyd. C6H6 added dropwise, the mixt. heated on a steam bath 3 hrs., and the product isolated as in the previous example to give 4-piperidino-2-butynyl diphenylisobutyrate-HCl, m. 156.5-8.5° (C6H6). To a soln. of 9.5 g. Me α-methylthiodiphenylacetate and 4.9 g. II in 150 ml. n-heptane was added about 50 mg. NaOMe, the mixt. stirred and refluxed, the MeOH-n-heptane azeotrope collected to a total of 0.85 ml. (addnl. NaOMe added during the distn.), the mixt. cooled and poured onto crushed ice-water, the org. layer sepd., washed with water, and extd. with 2N HCl, and the acidic exts. washed with Et2O and made alk. with 10% NaOH. The free base was taken up in Et2O, the soln. washed with water, dried (MgSO4), and filtered, and dry HCl passed in to give 5.4 g. 4-pyrrolidino-2-butynyl-α-methylthiodiphenylacetate-HCl, m. 154-6° (iso-PrOH). Similarly prepd. were (HCl salt m.p. given): 4-morpholino-2-butynyl benzilate, 158-60°; 4-diethylamino-2-butynyl-α-methylthiodiphenylacetate, 146-8° 4-piperidino-2-butynyl α-methylthiodiphenylacetate, 171.5-73°; 4-morpholino-2-butynyl α-methylthiodiphenylacetate, 171-3.5°; 4-diethylamino-2-butynylphenyl-α-thienylglycolate (81.5-3.5°), 4-diethylamino-2-butynyl phenylcyclohexylglycolate, 129-30°; 4-dimethylamino-2-butynyl benzilate, 130-3°; 4-diethylamino-2-butynyl benzilate, 128.5-30.5°; 4-piperidino-2-butynyl benzilate, 141.5-4°; 4-piperidino-2-butynyl α-methoxydiphenylacetate, 170.5-72°; and 4-piperidino-2-butynyl α-ethoxydiphenylacetate, 173.5-75°. A mixt. of 394.2 g. Me phenylcyclohexylglycolate and 293.1 g. 4-diethylamino-2-butynyl acetate was dissolved in 2.6 l. n-heptane by warming, the soln. heated with stirring to 60-70°, 8.0 g. NaOMe added, the temp. raised until the solvent distd., the distn. continued until no more MeOAc distd., the mixt. cooled to room temp., washed with water, and extd. with 165 ml. 2N HCl, the aq. exts. stirred to permit crystn. of the HCl salt, and crystn. completed by cooling to give 323 g. 4-diethylamino-2-butynyl phenylcyclohexylglycolate-HCl. A mixt. of 11.4 g. α-chlorodiphenylacetyl chloride and 4.9 g. 4-dimethylamino-2-butynol was heated 25 min. at 100-5°, then 30 min. at 70°, the oil washed thoroughly with anhyd. Et2O and dissolved in 100 ml. anhyd. EtOH, the soln. refluxed 25 hrs. with 5 g. Na2CO3, the mixt. cooled, filtered, and made basic with 10% NaOH, most of the EtOH removed in vacuo, the aq. mixt. extd. with Et2O, the exts. washed with water and dried over MgSO4, and then anhyd. HCl passed into the Et2O soln. to give 4.0 g. 4-dimethyl-2-butynyl α-ethoxydiphenylacetate-HCl, m. 166.5-8.5°.

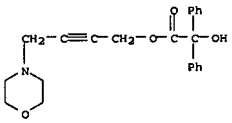
IT 3512-36-5P, Acetic acid, (methylthio)diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride 14597-23-0P, Benzilic acid, 4-morpholino-2-butynyl ester 95130-66-8P, Benzilic acid, 4-morpholino-2-butynyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 3512-36-5 CAPLUS
CN Acetic acid, (methylthio)diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI, 8CI) (CA INDEX NAME)

L4 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

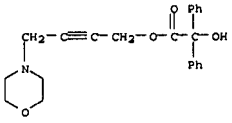


● HCl

RN 14597-23-0 CAPLUS
CN Benzilic acid, 4-morpholino-2-butynyl ester (7CI, 8CI) (CA INDEX NAME)



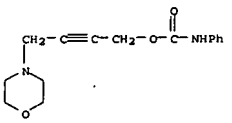
RN 95130-66-8 CAPLUS
CN Benzilic acid, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

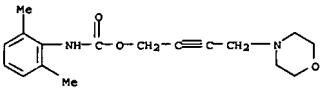
L4 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:448342 CAPLUS
DOCUMENT NUMBER: 59:48342
ORIGINAL REFERENCE NO.: 59:8730b-d
TITLE: Acetylene compounds of potential pharmacological value. II. 4-Amino-2-butynyl esters of phenylcarbamic acids.
AUTHOR(S): Dahlbom, Richard; Mollberg, Rene
CORPORATE SOURCE: Roy. Inst. Pharm., Stockholm
SOURCE: Acta Chemica Scandinavica (1963), 17, 1182-3.
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Et 2-chloro-6-methylphenylcarbamate (107 g.) was distilled in vacuo with P2O5 (142 g.) to give 60 g. 2-chloro-6-methylphenylisocyanate, b10 84-5°, n23D 1.5548. The appropriate phenylisocyanate (0.05 mole) and 0.05 mole IV were refluxed 3 hrs. in 25 ml. C6H6. The solution was cooled, diluted with Et2O, treated with ethereal HCl, and the precipitate was recrystd. (Et2O-EtOH) and dried at 50°/0.05 mm. to give X. The following X were prepared (R1 R2, R, % yield, and m.p. given): H, H, V, 50, 160.5-1.5°; Me, Me, V, 72, 182.5-3.5°; Me, Cl, V, 86, 171.2-2.5° (decomposition); H, H, VI, 54, 129.5-30.5°; Me, H, VI, 82, 129.5-31.0°; Me, Me, VI, 61, 175.5-6.5°; Me, Cl, VI, 86, 168-70° (decomposition); H, H, VII, 68, 148.5-9.5°; Me, H, VII, 79, 147.5-8° (decomposition); Me, Me, VII, 62,194-4.5° (decomposition); Me, Cl, VII, 77, 184.5-5° (decomposition); H, H, VIII, 65, 174.5-5.5°; Me, H, VIII, 57, 177-8° (decomposition); Me, Me, VIII, 80, 192.5-3° (decomposition); Me, Cl, VIII, 77, 177-8° (decomposition); H, H, IX, 78, 152.5-3°; Me, H, IX, 84, 173.5-4.5° (decomposition); Me, Me, IX, 73, 225-6° (decomposition); Me, Cl, IX, 75, 212-13° (decomposition).
IT 97417-91-9P, 2-Butyn-1-ol, 4-morpholino-, carbanilate, hydrochloride 98075-12-8P, Carbanilic acid, 2,6-dimethyl-, 4-morpholino-2-butynyl ester, hydrochloride 98222-92-5P, Carbanilic acid, 2-chloro-6-methyl-, 4-morpholino-2-butynyl ester, hydrochloride 98249-62-8P, Carbanilic acid, o-methyl-, 4-morpholino-2-butynyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)
RN 97417-91-9 CAPLUS
CN 2-Butyn-1-ol, 4-morpholino-, carbanilate, hydrochloride (7CI) (CA INDEX NAME)

L4 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



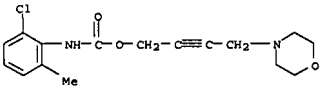
● HCl

RN 98075-12-8 CAPLUS
CN Carbanilic acid, 2,6-dimethyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

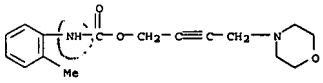
RN 98222-92-5 CAPLUS
CN Carbanilic acid, 2-chloro-6-methyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 98249-62-8 CAPLUS
CN Carbanilic acid, o-methyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)

L4 ANSWER 29 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

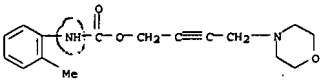
L4 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1963:448341 CAPLUS
DOCUMENT NUMBER: 59:48341
ORIGINAL REFERENCE NO.: 59:8729h,8730a-b
TITLE: Acetylene compounds of potential pharmacological value. I. 4-Amino-2-butynyl esters of diphenylacetic acid, 1-phenylcyclopentane-1-carboxylic acid, and phenothiazine-10-carboxylic acid
AUTHOR(S): Dahlbom, Richard; Mollberg, Rene
CORPORATE SOURCE: Roy. Inst. Pharm., Stockholm
SOURCE: Acta Chemica Scandinavica (1963), 17, 916-20
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Esters of diphenylacetic acid (I), 1-phenylcyclopentane-1-carboxylic acid (II), and phenothiazine-10-carboxylic acid (III) with RCH2C.tplbond.CCH2OH (IV) have been prepared, where R = NMe2 (V), NEt2 (VI), pyrrolidino (VII), piperidino (VIII), and morpholino (IX). IV was obtained from ClCH2C.tplbond.CCH2OH and the appropriate amine by the method of Biel (B., et al., CA 52, 6335g). Reported were IV (R, % yield, b.p./mm., and n22D given): VII, 85, 112-13°/0.9, 1.5092; VIII, 71, 101-2°/0.4, 1.5043. A solution of 0.055 mole acid chloride, 0.05 mole IV, and 0.06 mole Et3N in 50 ml. C6H6 was refluxed 3-20 hrs., then cooled, filtered, and concentrated in vacuo. The residue was dissolved in 50 ml. Et2O, treated with HCl and the precipitate recrystd. from Et2O-EtOH. Quaternary salts of III esters were also prepared The following RCH2C.tplbond.CCH2R1R2X were obtained (RH, R1, R2X, % yield, and m.p. given): III, V, HCl, 48, 185-6° (decomposition); III, V, EtBr, 83, 158-9° (decomposition); III, VI, HCl, 61, 181-2° (decomposition); III, VI, MeBr, 91, 141-2° (decomposition); III, VII, HCl, 69, 155.5-6.5° (decomposition); III, VII, MeBr, 89, 163-4° (decomposition); III, VIII, HCl, 72, 176-7° (decomposition); III, VIII, MeBr, 98, 170-1° (decomposition); III, IX, HCl, 64, 188-9° (decomposition); II, V, HCl, 86, 144-6°; II, VI, HCl, 57, 92.5- 4°; II, VIII, HCl, 65, 124-6°; II, IX, HCl, 71, 167-9°; I, VI, HCl, 79, 128-30°; I, VII, HCl, 83, 142-4°; I, VIII, HCl, 78, 158-60°; I, IX, HCl, 80, 160-1.5°.

IT 97417-91-9 98075-12-8 98222-92-5 98249-62-8
(Derived from data in the 7th Collective Formula Index (1962-1966))

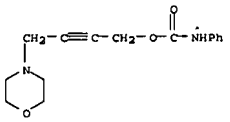
RN 97417-91-9 CAPLUS
CN 2-Butyn-1-ol, 4-morpholino-, carbanilate, hydrochloride (7CI) (CA INDEX NAME)

L4 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



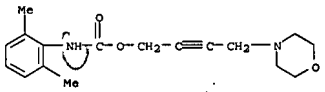
● HCl

L4 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



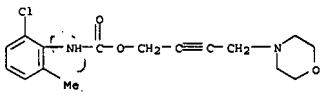
● HCl

RN 98075-12-8 CAPLUS
CN Carbanilic acid, 2,6-dimethyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 98222-92-5 CAPLUS
CN Carbanilic acid, 2-chloro-6-methyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

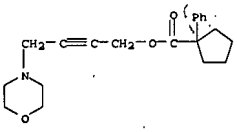
RN 98249-62-8 CAPLUS
CN Carbanilic acid, o-methyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)

L4 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

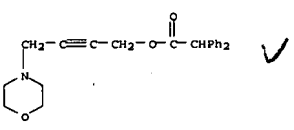
IT 17781-98-5P, Cyclopentanecarboxylic acid, 1-phenyl-, 4-morpholino-2-butynyl ester, hydrochloride 95130-43-1P, Acetic acid, diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride 101318-97-2P, Phenothiazine-10-carboxylic acid, 4-morpholino-2-butynyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)

RN 17781-98-5 CAPLUS
CN Cyclopentanecarboxylic acid, 1-phenyl-, 4-morpholino-2-butynyl ester hydrochloride (7CI, 8CI) (CA INDEX NAME)



● HCl

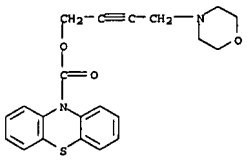
RN 95130-43-1 CAPLUS
CN Acetic acid, diphenyl-, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

L4 ANSWER 30 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 101318-97-2 CAPLUS
CN Phenothiazine-10-carboxylic acid, 4-morpholino-2-butynyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

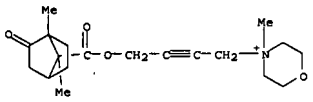
L4 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:24081 CAPLUS
DOCUMENT NUMBER: 55:24081
ORIGINAL REFERENCE NO.: 55:4777f-g
TITLE: Pharmacological studies on terpenes
AUTHOR(S): Nishio, Hyoe
CORPORATE SOURCE: Med. Coll., Nara
SOURCE: Nippon Yakurigaku Zasshi (1959), 55, 1552-67
CODEN: NYKZAU; ISSN: 0015-5691
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The ganglionic blocking activities of terpenes containing quaternary ammonium radicals were studied. Introduction of isoketopinic acid group to 2-morpholinoethanol-MeI was effective not only in the potentiation but in the prolongation of the ganglionic blocking action of the morpholinium compound Ketopinic acid derivs. demonstrated but a transient blocking action. They were destroyed by human serums and guinea pig liver homogenates. On the other hand, isoketopinic acid derivs. and π-oxocamphor oxime derivs. were not destroyed, and showed a marked prolonged effect.

IT 111357-35-8
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 111357-35-8 CAPLUS

CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium iodide, 1,7-dimethyl-2-oxo-7-norbornancarboxylate (6CI) (CA INDEX NAME)



● I⁻

L4 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:22847 CAPLUS
DOCUMENT NUMBER: 55:22847
ORIGINAL REFERENCE NO.: 55:4540a-c
TITLE: Aminoalkynyl N-alkylpiperidinecarboxylates
INVENTOR(S): Biel, John H.
PATENT ASSIGNEE(S): Lakeside Laboratories, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

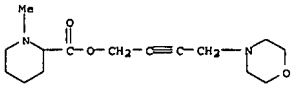
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2867619		19590106	US 1956-620165	19561105

AB The title compds. RN.(CH2)4.CHCO2(CH2)nC.tplbond.C(CH2)nNR1R2 (I) when quaternized are useful as anti-hypertensive and ganglion-blocking agents. Morpholine (87 g.) in 135 cc. benzene was treated dropwise with a solution of 41.8 g. 4-chloro-2-butyn-1-ol in 75 cc. benzene. After the exothermic reaction, the mixture was refluxed 3 hrs., cooled, filtered and distilled to give 90.8% 4-morpholino-2-butyn-1-ol (I), b0.01 104-6°. Me 2-(1-methylpiperidyl)carboxylate (31.4 g.), 31 g. I, and 0.5 g. NaOMe in 325 cc. heptane were heated and MeOH separated using a Dean-Stark tube to give 74.3% 4-morpholino-2-butynyl N-methylpipecolinate, b0.25 149-51° (short column); MeBr salt, m. 208-10°, yield 88.5%. Below are given other I prepared (R, NR1R2, % yield, b.p., n25D, and % yield and m.p. of the MeBr derivs. given): Me, NMe2, 70.2, b0.35 107-9°, 1.4824, 95.3, 193° (decomposition); Me, Et2N, 29.5, b0.5 133-5°, 1.4824, 60.4, 204-5° (decomposition); Me, pyrrolidino, 70.3, b0.55 138-9°, 1.4972, 98, 205° (decomposition); Me, morpholino, 74.3, b0.25 149-51°, 1.5012, 88.5, 208-10° (decomposition).

IT 101261-21-6
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 101261-21-6 CAPLUS

CN Pipecolic acid, 1-methyl-, 4-morpholino-2-butynyl ester (6CI) (CA INDEX NAME)

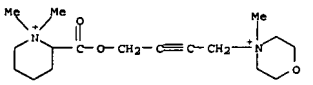


IT 109563-64-6P, 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with 2-carboxy-1,1-dimethylpiperidinium bromide
RL: PREP (Preparation)
(preparation of)

RN 109563-64-6 CAPLUS

CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with

L4 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
2-carboxy-1,1-dimethylpiperidinium bromide (6CI) (CA INDEX NAME)



●2 Br⁻

L4 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:22846 CAPLUS
DOCUMENT NUMBER: 55:22846
ORIGINAL REFERENCE NO.: 55:4539i,4540a
TITLE: 2-Chloropyridine 1-oxide
INVENTOR(S): Shermer, David A.
PATENT ASSIGNEE(S): Olin Mathieson Chemical Corp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

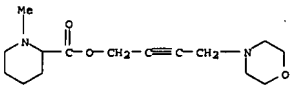
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2951844		19600906	US 1958-772008	19581105

AB AcO2H (0.51 mole) as a 40% aqueous solution was added over 15 min. to 1 mole 2-chloropyridine (I) at 70°, the mixture stirred 150 min. at 70°, neutralized with NaOH, and the unreacted I distilled at about 115° with H2O. The distillate separated into 2 phases; 0.61 mole I was recovered by decantation, to leave a residue of 0.39 mole 2-chloropyridine 1-oxide (100 and 77% yields, based on I and AcO2H, resp.). The recovered I was recycled.

IT 101261-21-6
(Derived from data in the 6th Collective Formula Index (1957-1961))

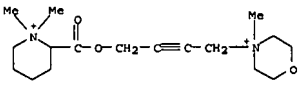
RN 101261-21-6 CAPLUS

CN Pipecolic acid, 1-methyl-, 4-morpholino-2-butynyl ester (6CI) (CA INDEX NAME)



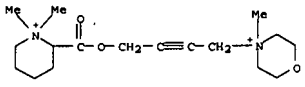
L4 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:7981 CAPLUS
DOCUMENT NUMBER: 55:7981
ORIGINAL REFERENCE NO.: 55:1539h-i,1540a-d
TITLE: Structure and reactions of gossypol
AUTHOR(S): Shirley, David A.
CORPORATE SOURCE: Univ. of Tennessee, Knoxville
SOURCE: Proc. Conf. Chem. Structure Reactions Gossypol Nongossypol Pigments Cottonseed, New Orleans (1959) 34-43
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB Gossypol (I) anils were prepared from a series of aliphatic and aromatic amines to study the scope of the reaction and to prepare derivs. of I to be used as (a) intermediates, (b) physiol. active compds., (c) dyes, or (d) model compds. for complexes of I with proteins. In group (a) were allylamine, diethylenetriamine, n-C18H37NH2, aminoacetal, p-H2NC6H4Ac, p-nitrobenzylamine, and p-BrC6H4CH2NH2, in group (b) H2NCH2CH2NMe2, p-H2NC6H4CO2Bu, p-H2NC6H4SO2NH2, and H2NCH2CH2Ph, in group (c) 4-(o-tolylazo)-o-toluidine and p-H2NC6H4N:NPh, and in group (d) H2NCH2CO2Me, DL-lysine Me ester, and H2NCH2CONHCH2CO2Me. Deapogossypol hexa-Me ether was demethylated with C5H5N.HCl to deapogossypol, which was converted to the hexaacetate, deapogossypolone tetraacetate, and deaphydrogossypolone octaacetate. Anhydrogossypol was treated with cyclopentadiene to give a crystalline product of proposed structure II. Apogossypol was converted to the hexaallyl ether, which was heated in a mixture of Me2NPh and Ac2O to give the tetraacetate of a partly rearranged product. I was oxidized in 10% aqueous NaOH with 30% aqueous H2O2 at 60-70° 8 min. to yield 2 crystalline compds., m. 231-3°, not further examined, and, m. 184-6°, tentatively identified by infrared and C-H analysis as 2,2'-dihydroxy-4,4'-diisobutyl-6,6'-dimethyl-biphenyl-3,3'-dicarboxylic acid (III); bis(2,4-dinitrophenyl hydrazide) m. 269-70°. Ac2O with III gave a diacetate. A possible mechanism for the formation of III was given.
IT 109563-64-6
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109563-64-6 CAPLUS
CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with 2-carboxy-1,1-dimethylpiperidinium bromide (6CI) (CA INDEX NAME)

L4 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



●2 Br⁻

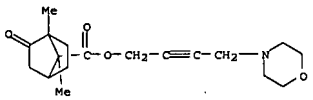
L4 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1961:7980 CAPLUS
DOCUMENT NUMBER: 55:7980
ORIGINAL REFERENCE NO.: 55:1539f-h
TITLE: β-Aroylpropionic acids. XVII. Establishment of the structure of β-(2-hydroxy-p-toluoyl)propionic acid
AUTHOR(S): El-Abbady, A. M.; Baddar, F. G.; Labib, A.
CORPORATE SOURCE: Ain-Shams Univ., Cairo
SOURCE: Journal of the Chemical Society (1960) 3420-1
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 55:7980
AB cf. CA 54, 22614i. The structure of β-(2-hydroxy-4-toluoyl)propionic acid (I), previously assumed on the basis of incomplete evidence (cf. Raval, et al., CA 33, 3779), was confirmed on the basis of the following reactions. I (5 g.) boiled 12 hrs. with 12 g. Me2SO4, 30 g. anhydrous K2CO3, and 15 ml. acetone gave 83% methyl β-(2-methoxy-4-toluoyl)propionate (II), m. 65-6° (C6H6-petr. ether). II (5.1 g.) boiled 2 hrs. with 3% alc. KOH gave 4.4 g. β-(2-methoxy-4-toluoyl)propionic acid (III), m. 127-8° (C6H6). III (1 g.), 40 ml. 3% KOH, and 3 g. KMnO4 heated 1 hr. on a boiling H2O-bath gave 0.6 g. 2-methoxyterephthalic acid. III (2 g.) reduced by the Martin modified Clemmensen method (30 hrs. at reflux) gave 1.8 g. γ-(2-methoxy-4-tolyl)butyric acid (IV), m. 54-5° (petr. ether). IV (1 g.) refluxed 2 hrs. with 0.5 ml. POCl3 in 10 ml. tetrachloroethane, and the mixture hydrolyzed with cold H2O and then steam-distilled gave 5-methoxy-7-methyl-1-tetralone; 2,4-dinitrophenylhydrazone, m. 223-4° (HOAc).
IT 109563-64-6
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 109563-64-6 CAPLUS
CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with 2-carboxy-1,1-dimethylpiperidinium bromide (6CI) (CA INDEX NAME)



●2 Br⁻

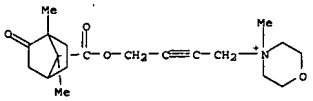
L4 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:34403 CAPLUS
DOCUMENT NUMBER: 54:34403
ORIGINAL REFERENCE NO.: 54:6789h-i,6790a-d
TITLE: Camphor derivatives as the ganglionic blocking agents.
I. Isoketopinic acid derivatives
AUTHOR(S): Nakanishi, Michio
CORPORATE SOURCE: Yoshitomi Pharm. Inds., Ltd., Fukuoka-ken
SOURCE: Yakugaku Zasshi (1959), 79, 1359-63
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB Na (1 mole) in liquid NH3 treated with 1 mole dialkylamino alc., the NH3 replaced with 10 vols. PhMe, the solution treated with 1 mole isoketopinoyl chloride, heated 1 hr. at 100°, cooled, the PhMe layer washed with NaHCO3, and the product distilled in vacuo gave dl-dialkylaminoalkyl isoketopinate (I). Me isoketopinate (1 mole) in 10 vols. heptane heated 2 hrs. with 1.5 moles dialkylamino alc. and 0.1 mole MeONa, the solvent removed, the residue in C6H6 extracted with 5% HCl, the HCl layer neutralized, and the oily product distilled gave I. I (1 mole) in C6H6 and 1.2 moles alkyl halide refluxed 5-7 hrs. and the product recrystd. (EtOH or Me2CO) gave I alkyl halide salt (II). I prepared were (dialkylaminoalkyl group, b.p./mm., m.p. of I.HCl, and m.p. of I alkyl halide salt given): Et2NCH2CH2, 160°/2, 145°, EtI, 152°; Me2N(CH2)3, 171-3°/3, 162°, MeI, 181°; Me2NCH2CH2, 142-6°/2, 191°, MeI, 208°; Et2N(CH2)3, 155-7°/2, 167°, -, -; RCH2CH2(R = morpholino), 203°3, 202°, MeI, 239° (BrCH2C.tplbond.CH salt m. 105°); R1CH2CH2 (R1 = piperidino), 170-6°/2, 247°, MeI, 280°; R(CH2)3, 185-90°/2, 209°, MeI, 205°; R1(CH2)3, 180-5°/2, 203°, MeI, 190°; RCH2CHMe, 150-7°/0.5, 183°, MeI, 208°; 4-ethoxyisoketopinoylpiperidinoethyl (III), 94°/0, 269°, MeI, 193°; RCH2C.tplbond.CCH2, 170°/0.07, 165°, MeI, 85°; R(CH2)4, 190-5°/0.9,103°, MeI, 65°. dl-Morpholinoethyl 3-chloroisoketopinate b0.6 172°; methiodide m. 232°. Dialkylaminoalkylamine (1 mole), 1 mole isoketopinoyl chloride in 5 vols. CHCl3, and 1 mole C5H5N refluxed 3 hrs., the CHCl3 layer extracted with 5% HCl, the HCl layer neutralized and the product recrystd. (C6H6) gave dl-N-isoketopinoyl-ω-dialkylaminoalkylamine (IV). IV (1 mole) in 10 vols. C6H6 heated with 1.2 moles MeI and the product recrystd. (EtOH) gave IV.MeI. IV prepared were (dialkylaminoalkyl group, m.p., m.p. of IV.HCl, and m.p. of IV.MeI given): 4-(2-hydroxyethyl)piperidino, 85°, 263°, 255°; Me2NCH2CH2, 48° 226°, 208°; Me2N(CH2)3, 85°, 209°, 250°; Et2N(CH2)3, 59°, 174°, 180°; R(CH2)3, 97°, 214°, 115°. I.MeI and hypotensive action (+ or ++) were (dialkylaminoalkyl group and activity given): Et2NCH2CH2, +; Me2N(CH2)3, +; Me2NCH2CH2, -; RCH2CH2, ++ (CH.tplbond.CCH2Br salt, ++); R1CH2CH2, ++; R(CH2)3, ++.
IT 101865-08-1 111357-35-8
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 101865-08-1 CAPLUS
CN 7-Norbornanecarboxylic acid, 1,7-dimethyl-2-oxo-, 4-morpholino-2-butynyl ester, hydrochloride (6CI) (CA INDEX NAME)

L4 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



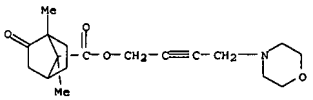
● HCl

RN 111357-35-8 CAPLUS
CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium iodide, 1,7-dimethyl-2-oxo-7-norbornancarboxylate (6CI) (CA INDEX NAME)

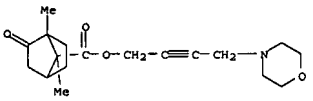


● I-

IT 101865-09-2P, 2-Butyn-1-ol, 4-morpholino-, 1,7-dimethyl-2-oxo-7-norbornanecarboxylate
RL: PREP (Preparation)
(preparation of)
RN 101865-09-2 CAPLUS
CN 7-Norbornanecarboxylic acid, 1,7-dimethyl-2-oxo-, 4-morpholino-2-butynyl ester (6CI) (CA INDEX NAME)

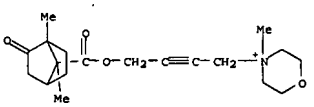


L4 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

RN 111357-35-8 CAPLUS
CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium iodide, 1,7-dimethyl-2-oxo-7-norbornancarboxylate (6CI) (CA INDEX NAME)



● I-

L4 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1960:34402 CAPLUS
DOCUMENT NUMBER: 54:34402
ORIGINAL REFERENCE NO.: 54:6789e-h
TITLE: Initiators and peroxide products of the liquid phase autoxidation of 3-carene
AUTHOR(S): Erofeev, B. V.; Chirko, A. I.
SOURCE: Uchenye Zapiski, Belorus. Gosudarst Univ. im. V. I. Lenina, Ser. Khim. (1956), 29, 15-22
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The primary product of the autoxidn. of 3-carene (I) was I hydroperoxide (II). On reduction, II gave carenol. The other product of the autoxidn. was 2,2'-peroxide (III) of I. The following initiators were investigated: MnO, MnO2, Mn(HCO2)2 (IV), Mn(OAc)2 (V), Mn butyrate (VI), Mn stearate (VII), Fe2O3, Co3O4, (HCO2)2Co (VIII), Co(OAc)2 (IX), Co butyrate (X), Co stearate (XI), Co oxalate (XII), MoO3, WO3, PbO2, the hydrate of lead oxide (XIII), Pb(OAc)2 (XIV), SeO2, kaolin (XV), and montmorillonite (XVI). The best initiators were: MnO2, Fe2O3, Co3O4, MoO3, WO3, PbO2, XV, XVI. Weak initiators were XII, XIII, and XIV. SeO2 had an inhibiting effect. In the case of MnO, IV, VIII, XII, WO3, XIII, XIV, XV, or XVI, the amount of II found among the products of the autoxidn. approached the % autoxidn.; in the case of strong initiator, the amount of II was smaller. I (35 g.) was oxidized in the presence of 1% XIV as long as the velocity of the oxidation began to decrease (4 l. O was necessary). The unchanged I was distilled and the residue fractionated 3 times in vacuo to give 8.5 g. II, b0.024 49-50°, d20 1.0117, n20D 1.4991, MR 48.79, did not react with 2,4-dinitrophenylhydrazine, reacted violently with Pb(OAc)4 (XVII). The distillation residue of II contained III, b0.06 100°, d20 1.0717, n20D 1.5150, n50D 1.5050, gave no reaction with XVII. On reduction by KI in AcOH II yielded carenol, b0.6 65-6°, d20 0.9892, n20D 1.4957, reacted with Na; phenylurethan m. 121°.
IT 101865-08-1 111357-35-8
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 101865-08-1 CAPLUS
CN 7-Norbornanecarboxylic acid, 1,7-dimethyl-2-oxo-, 4-morpholino-2-butynyl ester, hydrochloride (6CI) (CA INDEX NAME)

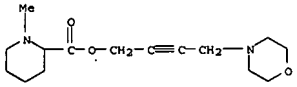
L4 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1958:35237 CAPLUS
DOCUMENT NUMBER: 52:35237
ORIGINAL REFERENCE NO.: 52:6335g-i,6336a-d
TITLE: Hypotensive agents. II. Aminoalkyl esters of piperidinecarboxylic acids and their "reversed" ester derivatives
AUTHOR(S): Biel, John H.; Sprengeler, Edwin P.; Friedman, Harris L.
CORPORATE SOURCE: Lakeside Labs., Inc., Milwaukee, WI
SOURCE: Journal of the American Chemical Society (1957), 79, 6184-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:35237
AB cf. C.A. 50, 2579d. Morpholine (87.0 g.) in 135 cc. C6H6 treated rapidly dropwise with 41.8 g. ClCH2C.tplbond.CCH2OH in 75 cc. C6H6, refluxed 3 hrs., cooled, and filtered, the residue washed with C6H6, and the combined filtrates distilled yielded 56.3 g. 4-morpholino-2-butyn-1-ol (I), viscous oil, b0.1 104-6°, n25D 1.5087. Me N-methylpipecolinate (31.4 g.) and 31.0 g. I in 325 cc. heptane refluxed with 0.5 g. NaOMe under a Dean-Stark trap in which the liberated MeOH seps. from the heptane (2 addnl. 0.3-g. portions NaOMe may be required to complete the reaction), 50% of the heptane distilled, and the residue chilled, filtered, and distilled gave 41.6 g. 4-morpholino-2-butynyl N-methylpipecolinate (II), b0.25 149-51°, n25D 1.5012. II (14.0 g.) in 80 cc. iso-PrOH refluxed 3 hrs. with 19.0 g. MeBr, cooled, and filtered yielded 20.8 g. II.2MeI, m. 208-10° (decomposition) (hot EtOH). Similarly were prepared the following aminoalkyl esters of 1-methylnipecotic acid (aminoalkyl group, b.p./mm. of ester, and m.p. of dimethobromide given): Me2N(CH2)2, 103-5°/4.0, 230-2°; Me2N(CH2)3, 106-9°/1.0, 238-9°; 2-morpholinoethyl, 116-20°/1.0, 235-6°; 2-pyrrolidinoethyl, 103-5°/1.0, 209-11°; o-ClC6H4CH2MeN(CH2)2, 148-53°/0.15, - (dimethiodide, 178-9°); 2-diethylaminoethyl 1-ethylnipecotinate, 104-6°/2.0, 221-2°. 3-Dimethylamino-2-propyl 1-methylnipecotinate, 137-41°/17, 255-7°; 2-dimethylaminoethyl isonipecotinate, 95-6°/1.0, 276-7°. The following aminoalkyl esters of 1-methylpipecolinic acid (same data given): Me2N(CH2)2, 145-7°/23,245°; Me2N(CH2)3, 156-8°/23, - (dimethiodide, 224-6°); 2-morpholinoethyl, 136-8°/1.2, 233-5°; o-ClC6H4CH2MeN(CH2)2, 100-5°/0.5, - (dimethiodide, 185°); 3-morpholinopropyl, 140-2°/0.8, - (dimethiodide, 169-71°). 2-Dimethylaminoethyl nicotinate, 154-6°/19, 218-19°. The following 1,x-MeC5H9N(CH2)mO2C(CH2)nNR2 (III) (ring position, m, n, NR2, b.p./mm. of ester, and m.p. of dimethobromide or in parentheses of dimethiodide given): 2, 1, 2, morpholino, 140-1°/0.8, 188-9°; 3, 0, 2, pyrrolidino, 105-8°/0.3, (165-6°); 3, 0, 2, morpholino, 136-9°/0.7, (183-3°); 3, 0, 1, NMe2, 136-8°/16, 183-4°; 3, 0, 2, Me2N, 158-60°/37, (194-5°); 3, 1, 1, Me2N, 147-8°/22, 232-3°; 4, 0, 1, Me2N, 110-13°/8, 263-4°; 3, 0, 2, o-ClC6H4CH2MeN, -, (125°). 3-(N-o-Chlorobenzylpiperidyl)3-morpholinopropionate (IV), 178-88°/0.05, 88°;

L4 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
3-pyrrolidinopropionate analog of IV, 169-72°/0.05, 82-4°.
The following analogs of II (b.p./mm., n25D of ester, and m.p. of dimethobromide given): Me2N, 107-9°/0.35, 1.4824, 193°; Et2N, 133-5°/0.50, 1.4824, 204-5°; pyrrolidino, 138-9°/0.55, 1.4972, 205°. The % lowering of blood pressure with 1.0 mg./kg. intravenously and 10 mg./kg. orally in the normotensive dog and the duration of the effect are tabulated for the various bisquaternary compds. Several of the compds. displayed potent and sustained hypotensive properties. The structural features necessary for optimum hypotensive activity are discussed.

IT 101261-21-6P, 2-Butyn-1-ol, 4-morpholino-, 1-methylpipecolate
109563-64-6P, 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with 2-carboxy-1,1-dimethylpiperidinium bromide
RL: PREP (Preparation)
(preparation of)

RN 101261-21-6 CAPLUS

CN Pipecolic acid, 1-methyl-, 4-morpholino-2-butynyl ester (6CI) (CA INDEX NAME)



RN 109563-64-6 CAPLUS

CN 4-(4-Hydroxy-2-butynyl)-4-methylmorpholinium bromide, ester with 2-carboxy-1,1-dimethylpiperidinium bromide (6CI) (CA INDEX NAME)